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ONE-PARAMETER AND TWO-CONJUGATE PARAMETER FAMILIES OF GENERATOR STATES

by

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ABSTRACT

The properties of the subspaces of the many-body Hilbert space which are associated with the use of the Generator Coordinate Method (GCM) in connection with one parameter, and with two-conjugate parameter families of generator states are examined in detail. These families are obtained by letting unitary displacement operators, having as generators canonical operators $\hat{P}$ and $\hat{Q}$, defined in the many-body Hilbert space, act on a reference state. We show that natural orthonormal base vectors in each case are immediately related to Peierls-Yoccoz and Peierls-Thouless projections respectively. Through the formal consideration of a canonical transformation to collective, $\hat{P}$ and $\hat{Q}$, and intrinsic degrees of freedom, we discuss in detail the properties of the GCM subspaces with respect to the kinematical separation of these degrees of freedom. An application is made, using the ideas developed in this paper, a) to translations; b) to illustrate the qualitative understanting of the content of existing GCM calculations of giant ressonances in light nuclei and c) to the definition of appropriate asymptotic states in current GCM descriptions of scattering.

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I - INTRODUCTION

The generator coordinate method (GCM) provides a variational approximation to the dynamical behavior of quantum many-body systems which guarantees the linear completeness of the variational space. In fact the variational space of the GCM can always be associated with a projection operator, defined in the many-body Hilbert space, which can be constructed explicitly in terms of the adopted set of generator states[1,2]. Characteristic features resulting from the quantum superposition principle are thus preserved and this is the foundation of the fully quantum mechanical character of approximations based on the GCM[3,4]. In the GCM scheme the dynamical properties of the many-body system are determined by the projection of the many-body hamiltonian $\hat{H}$ onto the GCM variational subspace S, $\hat{S}\hat{H}\hat{S}$, where $\hat{S}$ is the projection operator associated with the GCM variational subspace S

$$\hat{S} = \hat{S}^{+} = \hat{S}^{2}$$

One of the distinguishing features of the GCM is the fact that the variational subspace S can be constructed with no reference to any collective dynamical variable. Indeed, the choice of the generator states is made on the basis of educated guesses as to the nature of the collective properties under consideration (see e.g. references 5, 15, 16 and 18). These generator states are put in one to one correspondence with the points $\vec{\alpha}$ of a label space. The labels $\vec{\alpha}$ are usually, but not necessarily, equal or related to the expectation values of some adequate dynamical variables of the many-body system under consideration. However once the GCM variational space (or equivalently the corresponding projection operator $\hat{S}$) is specified through a definite choice of generator states, one can find, a posteriori, natural dynamical variables in S . These natural dynamical variables allow us to describe the restricted dynamics of the many-body system in terms of a small number of spe ialized degrees of freedom.

The quantum mechanical character of the GCM does not stand by itself as a sufficient virtue, however. Restricting the problem to a subspace of the original many-body phase space brings about truncation effects that are in general difficult to assess. An obvious additional formal requirement, that the projection operator involved in the truncation should be as nearly as possible a constant of motion[1,2] seems to be of little guiding value when one is confronted with realistic problems. These difficulties stem, of course, from the fact that one is confronted here with a dynamical question that cannot be ultimately settled as such whitout reference to some specific hamiltonian. As we show in detail in this paper, however, this dynamical question can be, so to say, reduced to a "kinematical level" provided that collective dynamical variables associated with the relevant collective degrees of freedom is given in the many-body phase space $\mathcal{H}$. Here lies, of course, the dynamical part of the problem. What remains then to be done is to set up a GC scheme such that the resulting variational space is well adapted to the unfolding of the corresponding collective dynamics.

In order to clarify these ideas and gain some general operational expediency one may consider such matters from the following point of view. First, consider for definiteness the case of a canonical degree of freedom, i.e., a collective degree of freedom associated with a canonical pair suitably defined in the many-body Hilbert space $\mathcal{H}$

$$[\hat{Q},\hat{P}]=i$$

one can then introduce a canonical tranformation from the particle degrees of freedom $\hat{\vec{p}}_i$, $\hat{\vec{q}}_i$ to $\hat{P}$, $\hat{Q}$ and to additional intrinsic variables $\hat{\pi}_i$, $\hat{\xi}_i$ (i=1, 3A-1). At the same time we are naturally led to consider $\mathcal{H}$ as the direct product of a collective space $\mathcal{H}_C$ and an intrinsic space $\mathcal{H}_I$, i.e.

$$\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_I \tag{I.1}$$

We may also decompose the hamiltonian describing the systems as

$$\hat{H} = \hat{H}_c(\hat{P},\hat{Q}) + \hat{H}_I(\hat{\pi}_i,\hat{\xi}_i) + \hat{H}'(\hat{Q},\hat{P},\hat{\xi}_i,\hat{\pi}_i) \tag{I.2}$$

where the last term, $\hat{H}'$, represents the coupling between collective and intrinsic degrees of freedom. It is also useful to consider a subspace of the many-body Hilbert space, to be called the ideal collective subspace, which is given by the direct product of the collective space and a one-dimensional subspace of the intrinsic space:

$$\hat{S}_c\mathcal{H} = \mathcal{H}_c \otimes \hat{s}_I\mathcal{H}_I \tag{I.3}$$

In eq. (I.3) we introduced the projection operator onto the appropriate one-dimensional subspace of the intrinsic space $\mathcal{H}_I$

$$\hat{s}_I = \hat{s}_I^+ = s_I^2 = |I\rangle\langle I|$$

Thus

$$\hat{S}_c^+ = \hat{S}_c = \hat{S}_c^2 = \hat{1}_c \otimes \hat{s}_I$$

is the projection operator onto the ideal collective subspace. We may also consider the complementary projection operator

$$\hat{R}_c = \hat{1} - \hat{S}_c = \hat{1}_c \otimes (\hat{1}_I - \hat{h}_I)$$

In terms of these operators $\mathcal{H}$ can be written as the <u>direct sum</u> of two complementary spaces

$$\mathcal{H} = \hat{S}_c \mathcal{H} \oplus \hat{R}_c \mathcal{H}$$

while the hamiltonian $\hat{H}$ of the system under consideration can be decomposed as

$$\hat{H} = \hat{S}_c \hat{H} \hat{S}_c + \hat{R}_c \hat{H} \hat{R}_c + \hat{S}_c \hat{H} \hat{R}_c + \hat{R}_c \hat{H} \hat{S}_c \tag{I.4}$$

The last two terms represent the dynamical coupling of the subspaces.

The conditions for the systems to sustain a well developed collective mode can be stated in terms of a weak coupling limit, which in the case of the ideal collective mode implies that the last two terms in eq. (I.4) vanish. The eigenfunctions of $\hat{S}_c \hat{H} \hat{S}_c$ are then determined by the collective hamiltonian $\hat{H}_c(\hat{P}, \hat{Q})$, and the projectors $\hat{S}_c$ and $\hat{R}_c$ are constants of motion. The diagonalization of $\hat{S}_c \hat{H} \hat{S}_c$,

$$\hat{S}_c \hat{H} \hat{S}_c = \hat{S}_c \left(\hat{H}_c(\hat{P}, \hat{Q}) + \langle I | \hat{H}_I | I \rangle \right) \hat{S}_c$$

gives part of the exact energy spectrum of $\hat{H}$.

We may now ask how does the GCM variational subspace S stands with respect to the product space decomposition (I.3). In particular we can ask how does the GCM hamiltonian, $\hat{S}\hat{H}\hat{S}$, compares with $\hat{S}_c \hat{H} \hat{S}_c$. On a purely formal basis $\hat{S}\hat{H}\hat{S}$ can be split into three contributions,

$$\hat{S}\hat{H}\hat{S} = \hat{S}\hat{H}_c\hat{S} + \hat{S}\hat{H}_I\hat{S} + \hat{S}\hat{H}'\hat{S}$$

which originates respectively from each of the terms in eq. (I.2). We see thus that in general the GC dynamics can be ruled by the collective hamiltonian $\hat{H}_C$, by the purely intrinsic part $\hat{H}_I$ and by the coupling term $\hat{H}'$. Even in the case where $\hat{H}'$ vanishes the GC dynamics may still engage the instrinsic degrees of freedom through $\hat{S}\hat{H}_I\hat{S}$. The use of the GCM will thus in general give rise to a spurious "kinematical coupling" (i.e. resulting from the GC scheme and not from $\hat{H}$ which in this case does not couple the intrinsic and collective degrees of freedom) between the intrinsic and collective degrees of freedom. A typical manifestation of such a "kinematical coupling" (see section V) is the incorrect translational mass that one in general obtains when one uses the technique of Peierls-Yoccoz projection. This amounts in fact to a particular GCM treatment of the true translational motion of the system as a whole.

In order to obtain an adequate description of the collective dynamics in terms of the GCM , the construction of the variational space S , which we call in what follows the GCM collective subspace, must be such as to eliminate such spurious coupling effects. In this paper we show how this can be achieved once a collective canonical pair $\hat{P}$ and $\hat{Q}$ is adopted as relevant. Specifically, we discuss in detail the GCM collective subspace S generated by one and two parameter families of generator states obtained by letting unitary displacement operators having $\hat{P}$ and $\hat{Q}$ as generators act on a reference state. These spaces can be immediately related to Peierls-Yoccoz and to Peierls-Thouless projections respectively. This is done in section II. In section III we discuss the relationship between these two spaces and give conditions under which they are identical. Natural dynamical variables associated with specific representations in these spaces are defined in section IV where the expression of $\hat{S}\hat{H}\hat{S}$ in terms of these variables is also given. In section V we discuss in detail the separation of collective and intrinsic degrees of freedom in the framework of the GC dynamics and in section VI we illustrate the qualitative understanding that can be gained, using the ideas developed in this paper, of the content of existing GCM calculations of giant resonances in light nuclei. The significance of our results for the construction of asymptotic states in scattering theory is also shown. Section VII contains some concluding remarks.

II - A REPRESENTATION FOR THE GCM COLLECTIVE SUBSPACE

II.1 - ONE GENERATOR COORDINATE

We define the one parameter family of generator states (O.P.F.) as

$$|\alpha\rangle = e^{-i\alpha\hat{P}}|0\rangle \tag{II.1}$$

The ket $|0\rangle$ stands for a suitably chosen normalized reference or "fiducial" many-body state and $\hat{P}$ is a collective hermitian operator generating relevant changes of the reference state.

The overlap kernel $\langle\alpha|\alpha'\rangle$

$$\begin{aligned}\langle\alpha|\alpha'\rangle &= (\alpha|\hat{N}|\alpha') \\ &= \langle 0|e^{i(\alpha-\alpha')\hat{P}}|0\rangle\end{aligned} \tag{II.2}$$

depends only on the difference of the generator coordinates and so it can be diagonalized by a Fourier transform

$$\int_{-\infty}^{+\infty}(\alpha|\hat{N}|\alpha')(\alpha'|k)\,d\alpha' = 2\pi\Lambda(k)(\alpha|k) \tag{II.3}$$

The eigenfunctions and eigenvalues are respectively

$$\begin{aligned}(\alpha|k) &= \frac{1}{\sqrt{2\pi}}\,e^{ik\alpha} \\ \Lambda(k) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}d\alpha\,\langle\alpha|0\rangle\,e^{-ik\alpha} \\ &= \langle 0|\hat{\Pi}_k^{PY}|0\rangle\end{aligned} \tag{II.4}$$

and $\hat{\Pi}_k^{PY}$ is the Peierls-Yoccoz projection operator[6]

$$\hat{\Pi}_k^{PY} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\alpha \; e^{ik\alpha}\, e^{-i\alpha\hat{P}} \qquad \text{(II.5a)}$$

$$= \delta(\hat{P}-k)$$

The properties of the scalar product in the many-body Hilbert-space and the time reversal properties of $\hat{P}$ and $|o\rangle$ ($\hat{P}$ is a time odd operator and $|o\rangle$ a time even state) make $\Lambda(k)$ a semi-positive definitive even function of k . Besides one has from eqs. (II.4) and (II.5a)

$$\int_{-\infty}^{+\infty} dk\, \Lambda(k) = 1 \qquad \text{(II.5b)}$$

In what follows we assume that $\Lambda(k)$ decreases monotonicaly as a function of $|k|$, i.e., that $\Lambda(k)$ has a maximum at k equal to zero and decreases to zero at infinity. This hypothesis is not essential and it is made only to simplify the discussion. The general case is discussed in detail in reference 1.

Following reference 1 one can find a representation in the GCM collective subspace S_1 constructing base states in terms of the eigenfunctions of the overlap kernel $\langle\alpha|\alpha'\rangle$. In this case the projection operator in S_1 can be written as

$$\hat{S}_1 = \int_{-\infty}^{+\infty} dk\, |\psi_k\rangle_Y \, {}_Y\langle \psi_k|$$

The states $|\psi_k\rangle_Y$ form a continuous orthonormal base and they are given as

$$|\Psi_k\rangle_Y = \frac{1}{\sqrt{2\pi\Lambda(k)}} \int d\alpha\, |\alpha\rangle (\alpha|k)$$

$$= \frac{\hat{\Pi}_k^{PY}\, |0\rangle}{\sqrt{\langle 0|\hat{\Pi}_k^{PY}|0\rangle}} \qquad \text{(II.6)}$$

As shown by eq. (II.6) they are equal to normalized Peierls-Yoccoz projections of the reference state $|o\rangle$, associated with the operator $\hat{P}$. The representation found above is the specific representation given by the diagonalization of the overlap kernel. This is very convenient for sorting out the kinematical oddities inherent to the generator coordinate method but other representations may be prefereable from a physical point of view. Thus it is clear that a transformation theory in the subspace S_1 allows us to find, by an unitary transformation, another representation which diagonalizes any self-adjoint operator defined in S_1.

II.2 - TWO CONJUGATE GENERATOR COORDINATES

We define the two conjugate parameter family of generator states (T.C.P.F.) as

$$|\alpha,\beta\rangle = e^{-i\alpha\hat{P}}\, e^{i\beta\hat{Q}}\, |0\rangle \qquad \text{(II.7)}$$

where $\hat{P}$ and $\hat{Q}$ are conjugated collective operators in the many-body Hilbert space, i.e.,

$$[\hat{Q},\hat{P}] = i$$

The overlap kernel $\langle\alpha\beta|\alpha'\beta'\rangle$ is given by

$$\langle\alpha\beta|\alpha'\beta'\rangle = (\alpha\beta|\hat{N}|\alpha'\beta')$$

$$= \langle 0| e^{-i\beta\hat{Q}} e^{i(\alpha-\alpha')\hat{P}} e^{i\beta'\hat{Q}} |0\rangle \tag{II.8}$$

and its eigenfunctions and eigenvalues are determined by the equation

$$\int (\alpha\beta|\hat{N}|\alpha'\beta')(\alpha'\beta'|kn)\, d\alpha' d\beta' = 2\pi\, \lambda_n(k)(\alpha\beta|kn) \tag{II.9}$$

In appendix A we show that the eigenfunctions of $\langle\alpha\beta|\alpha'\beta'\rangle$ are

$$(\alpha\beta|kn) = \frac{e^{ik\alpha}}{\sqrt{2\pi}}\, \phi_n(\beta-k) \tag{II.10}$$

and that the eigenvalues $\lambda_n(k)$ are independent of k. The functions $\phi_n(\beta)$ and the λ_n are eigenfunctions and eigenvalues of the semi-positive definite Hilbert-Schmidt kernel

$$(\beta|\hat{n}|\beta') = \langle 0| e^{-i\beta\hat{Q}}\, \delta(\hat{P})\, e^{i\beta'\hat{Q}} |0\rangle \tag{II.11}$$

$$\int (\beta|\hat{n}|\beta')\, \phi_n(\beta')\, d\beta' = \lambda_n\, \phi_n(\beta) \tag{II.12}$$

The reduced kernel $(\beta|\hat{n}|\beta')$ can have zero eigenvalues and when they occur there are two important consequences. One is that the weight functions defined in the null space of $\hat{N}$ give rise to vectors of zero norm[†] in the many-body Hilbert space. Therefore there is no loss of generality if we restrict the weight function space to the orthogonal complement of the null space of $\hat{N}$. The other is that the existence of eigenvectors of $\hat{N}$ with zero eigenvalue implies that the generator states are not linearly independent, and the linear dependence is expressed by

$$|\alpha\beta\rangle = \int d\alpha' d\beta' \, |\alpha'\beta'\rangle \, R(\alpha'\beta';\alpha\beta) \tag{II.13}$$

where the kernel $R(\alpha\beta,\alpha'\beta')$ is

$$R(\alpha\beta;\alpha'\beta') = \sum_{n,\lambda_n \neq 0} \int dk \, (\alpha\beta|kn)(kn|\alpha'\beta') \tag{II.14}$$

which is seen to be equal to the projection operator on the orthogonal complement of the null space of $\hat{N}$.

As in the previous O.P.F. case we can find a representation for the GCM collective subspace S_2 in terms of eigenfunctions of the overlap kernel $\langle\alpha\beta|\alpha'\beta'\rangle$. In the T.C.P.F. case the projection operator in S_2 is given by

$$\hat{S}_2 = \sum_{n,\lambda_n \neq 0} \int dk \, |\Psi_{k,n}\rangle_T \, {}_T\langle\Psi_{k,n}| \tag{II.15}$$

where the base states are

$$\begin{aligned} |\Psi_{k,n}\rangle_T &= \frac{1}{\sqrt{2\pi\lambda_n}} \int d\alpha\, d\beta \, |\alpha\beta\rangle (\alpha\beta|kn) \\ &= \frac{\hat{\Pi}^{PT}_{k,n}|0\rangle}{\sqrt{\lambda_n}} \end{aligned} \tag{II.16}$$

In eq. (II.16) $\hat{\Pi}_{k,n}^{PT}$ is the so-called Peierls-Thouless double projection operator[6] .

$$\hat{\Pi}^{PT}_{k,n} = \int d\alpha\, d\beta \; \frac{e^{ik\alpha}}{2\pi} \, \phi_n(\beta-k) \, e^{-i\alpha\hat{P}} e^{i\beta\hat{Q}} \tag{II.17}$$

The states $|\psi_{k,n}\rangle_T$ are normalized as

$$_T\langle\psi_{k,n}|\psi_{k',n'}\rangle_T = \delta(k-k')\,\delta_{nn'}$$

and, as shown by eq. (II.16), they are equal to the normalized Peierls-Thouless projection of the reference state $|o\rangle$, associated with the operator $\hat{P}$. Furthermore they are labelled by two quantum numbers, one discrete, n, and other continuous, k. The number of discrete labels is equal to the number of eigenvectors of the reduced kernel with non-vanishing eigenvalues. As this kernel is of Hilbert-Schmidt type this number can be finite or infinite and in the last case λ_n has a single limit point at $\lambda=0$ (2).

The representation specified by eqs. (II.15) and (II.16) is the one obtained by the diagonalization of the overlap kernel and by unitary transformations in S_2 one can find other representation which diagonalizes any self-adjoint operator defined in S_2.

III - RELATIONSHIP BETWEEN THE SUBSPACES

The generator states $|\alpha\rangle$ and $|\alpha\beta\rangle$ are vectors defined in the GCM collective subspaces S_1 and S_2 respectively. Therefore we can find the projection of these states along the base states $|\psi_k\rangle_Y$ and $|\psi_{k,n}\rangle_T$. Using eqs. (II.3) and (II.6), and eqs. (II.9) and (II.16) one has

$$\langle\alpha|\Psi_k\rangle_Y = \sqrt{2\pi\Lambda(k)}\ (\alpha|k) \tag{III.1}$$

$$\langle\alpha\beta|\Psi_{k,n}\rangle_T = \sqrt{2\pi\lambda_n}\ (\alpha\beta|kn) \tag{III.2}$$

The generator states $|\alpha\rangle$ are moreover contained in the set $|\alpha\beta\rangle$ since $|\alpha\rangle = |\alpha,\beta = 0\rangle$. Then, using eq. (III.2) one has

$$\langle\alpha|\Psi_{k,n}\rangle_T = \sqrt{2\pi\lambda_n}\ (\alpha|k)\ \phi_n^*(k) \tag{III.3}$$

where we used the property

$$\phi_n^*(-p) = \phi_n(p)$$

which can be obtained by time revisal, $\hat{Q}$ being taken as a time-even operator.

Inserting eq. (III.3) into eq. (II.6) and (II.4) we can write the states $|\psi_k\rangle_Y$ as a linear superposition of the states $|\psi_{k,n}\rangle_T$,

$$|\Psi_k\rangle_Y = \sum_{n,\lambda_n\neq 0} V_n(k)\,|\Psi_{k,n}\rangle_T \tag{III.4}$$

where

$$V_n(k) = \frac{\sqrt{\lambda_n}\ \phi_n(k)}{\sqrt{\sum_{n,\lambda_n\neq 0} \lambda_n |\phi_n(k)|^2}}$$

which shows that

$$\sum_{n,\lambda_n\neq 0} |V_n(k)|^2 = 1 \tag{III.5}$$

The projection operators in the GCM collective subspaces generated by the one and two conjugate parameter family of generator states satisfy therefore the equations

$$\hat{S}_2 |\Psi_k\rangle_Y = |\Psi_k\rangle_Y \tag{III.6}$$

$$\hat{S}_1 |\Psi_{k,n}\rangle_T = V_n^*(k) |\Psi_k\rangle_Y \tag{III.7}$$

Eqs. (III.6) and (III.7) show that S_1 is always contained in S_2 , but that, in general, the converse is not true. S_2 is contained in S_1 only when the reduced kernel (II.11) has a single eigenvector with nonvanishing eigenvalue λ_0 .

In fact considering eq. (III.5) one has

$$|V_0(k)|^2 = 1 \tag{III.8a}$$

and the phases can be chosen such that

$$V_0(k) = 1 \tag{III.8b}$$

Thus eq. (III.7) becomes

$$\hat{S}_1 |\Psi_{k,0}\rangle_T = |\Psi_{k,0}\rangle_T$$

In this special case the two conjugate parameter family is redundant in the sense that it gives rise to the same collective subspace as the one parameter family. As a consequence of this redundancy the two-conjutate parameter family can be written as a linear superposition of the one parameter family since in this case the states $|\psi_k\rangle_Y$ are also a base in S_2. Thus, using eqs. (III.2), (III.4) and (II.6), we have

$$|\alpha\beta\rangle = \int d\alpha' \, |\alpha'\rangle \, T(\alpha'; \alpha\beta) \tag{III.9}$$

where

$$T(\alpha', \alpha\beta) = \int \frac{dk}{2\pi} \, e^{ik(\alpha'-\alpha)} \frac{\phi_0(k-\beta)}{\phi_0(k)}$$

It may still be advantageous to use the redundant two-conjugate parameter family since the generator states $|\alpha\beta\rangle$ have in this case very useful mathematical properties. As an example it can be easily shown that in this particular case the weight function always exists as a regular function and we can find a representation in the collective subspace which is diagonal in the generator coordinate states. We can view this particular case as a slight generalization of the concept of coherent states[7]. The property discussed above is called "global redundancy" in references 8 and 9. The concept of a "local redundancy", which is a particular case of global redundancy, is also introduced there. It corresponds to the fact that the action of $\hat{P}$ on the states $|\alpha\beta\rangle$ are equally expressed by the action of $\hat{Q}$ on $|\alpha\beta\rangle$, which in our case demands

$$i(\hat{P}-\beta)|\alpha\beta\rangle + \frac{(\hat{Q}-\alpha)}{b_0^2}|\alpha\beta\rangle = 0 \qquad \text{(III.10)}$$

where

$$b_0^2 = 2\langle 0|\hat{Q}^2|0\rangle$$

The eq. (III.10) holds only in the case where $|0\rangle$ is the vacuum of the boson operator

$$\hat{b} = \frac{1}{\sqrt{2}}\left(\frac{\hat{Q}}{b_0} + i\hat{P}b_0\right)$$

in which case $|\alpha\beta\rangle$ reduces to a coherent state.

IV - GCM COLLECTIVE OPERATORS

IV.1 - THE OPF CASE

The base states $|\psi_k\rangle_Y$ depending on a continuous label k, can be associated with a pair of canonical operators in S_1 defined by

$$\hat{P}_1 |\psi_k\rangle_Y = k |\psi_k\rangle_Y$$

$$\hat{Q}_1 |\psi_k\rangle_Y = -i\, \partial/\partial k\, |\psi_k\rangle_Y \tag{IV.1}$$

$$[\hat{Q}_1, \hat{P}_1] = i\, \hat{S}_1$$

The definitions (IV.1) yield

$$\hat{P}_1 = \int dk\, |\psi_k\rangle_Y\, k\, {}_Y\langle\psi_k|$$

$$\hat{Q}_1 = \int dk\, dk'\, |\psi_k\rangle_Y\, i\, \delta'(k-k')\, {}_Y\langle\psi_{k'}|$$

Thus $\hat{Q}_1$ and $\hat{P}_1$ are natural collective dynamical variables associated with the representation $\{|\psi_k\rangle_Y\}$, eq. (II.6).

Instead of using the representation given by eq. (II.6) directly, other representations may be prefereable. They can be found in general by unitary transformations in S_1. As an example the Fourier transforms of the states $|\psi_k\rangle_Y$

$$|\psi_x\rangle = \frac{1}{\sqrt{2\pi}} \int e^{-ikx} |\psi_k\rangle_Y \tag{IV.2}$$

define another base in S_1 in which the operator $\hat{Q}_1$ is diagonal

$$\hat{Q}_1 |\Psi_x\rangle = x |\Psi_x\rangle$$

$$\hat{P}_1 |\Psi_x\rangle = i \frac{\partial}{\partial x} |\Psi_x\rangle$$

Another representation is obtained by transforming (IV.2) by means of harmonic oscillator wave functions. This is a discrete representation which diagonalizes a boson number operator constructed from $\hat{P}_1$ and $\hat{Q}_1$.

The relationship between the GCM collective operators $\hat{Q}_1$ and $\hat{P}_1$ in the collective subspace S_1 and the collective operators $\hat{Q}$ and $\hat{P}$ in the full Hilbert space can be exhibited in the follwing way. Since $|\psi_k\rangle_Y$ is the Peierls-Yoccoz projection of the reference state $|o\rangle$, associated with the operator $\hat{P}$, one has by construction that

$$\hat{P} |\Psi_k\rangle_Y = k |\Psi_k\rangle_Y \tag{IV.3}$$

This equation shows that

$$\begin{aligned} \hat{P}_1 &= \hat{P}\hat{S}_1 \\ &= \hat{S}_1 \hat{P} \end{aligned} \tag{IV.4}$$

which, using the canonical commutation relations between $\hat{Q}$ and $\hat{P}$ gives

$$\hat{Q}_1 = \hat{S}_1 \hat{Q} \hat{S}_1 \tag{IV.5}$$

It can moreover be shown by a straightforward calculation that, in general

$$[\hat{Q}, \hat{S}_1] \neq 0 \tag{IV.6}$$

In sumary, this discussion shows first that the pair of canonical operators $\hat{P}_1$ and $\hat{Q}_1$ in S_1 are equal to the projection in S_1 of the canonical operators $\hat{P}$ and $\hat{Q}$ in the full Hilbert space; second, $\hat{P}$ is diagonal in the representation given by the orthonormal set of eq. (II.6); and finally, there is no representation of S_1 where $\hat{Q}$ is diagonal since the collective subspace S_1 is in general not an eigenspace of $\hat{Q}$.

IV.2 - THE TCPF CASE

The collective subspace generated by the T.C.P.F. has a base given by the states $|\psi_{k,n}\rangle_T$. These states have two quantum labels one continuous and the other discrete. In what follows we focus our attention on the continuous label. We could also use the discrete label n to define additional dynamical variables, commuting with those to be associated with the continuous label k , but for ease of presentation we defer this discussion until section V.

As in the O.P.F. case we define a pair of canonical operators in S_2 by

$$\begin{aligned} \hat{P}_2 |\psi_{k,n}\rangle_T &= k\, |\psi_{k,n}\rangle_T \\ \hat{Q}_2 |\psi_{k,n}\rangle_T &= -i\, \partial/\partial k\, |\psi_{k,n}\rangle_T \end{aligned} \tag{IV.7}$$

The definition (IV.7) leads to

$$\begin{aligned} \hat{P}_2 &= \sum_n \int dk\, |\psi_{k,n}\rangle_T\, k\, {}_T\langle\psi_{k,n}| \\ \hat{Q}_2 &= \sum_n \int dk\, dk'\, |\psi_{k,n}\rangle_T\, i\, \delta'(k-k')\, {}_T\langle\psi_{k',n'}| \end{aligned} \tag{IV.8}$$

The fact that $|\psi_{k,n}\rangle_T$ is the Peierls-Thouless projection of the reference state $|0\rangle$ associated with the operator $\hat{P}$ (see eq. (II.16)) gives now

$$\hat{P}|\psi_{k,n}\rangle_T = k\,|\psi_{k,n}\rangle_T$$
$$\hat{Q}|\psi_{k,n}\rangle_T = -i\,\partial/\partial k\,|\psi_{k,n}\rangle_T \tag{IV.9}$$

These equations yield

$$\hat{P}_\lambda = \hat{P}\hat{S}_2 = \hat{S}_2\hat{P}$$
$$\hat{Q}_\lambda = \hat{Q}\hat{S}_2 = \hat{S}_2\hat{Q}$$

Thus the canonical collective operators in S_2 are the projection in S_2 of the canonical collective operators in the full Hilbert space $\hat{Q}$ and $\hat{P}$. However, unlike in the O.P.F. case, here both operators commute with $\hat{S}_2$. Therefore the GCM collective subspace S_2 is an eigenspace of $\hat{Q}$, and by an unitary transformation in S_2 we can find a representation of S_2 where $\hat{Q}$ is diagonal. This can be achieved by means of a Fourier transform

$$|\psi_{x,n}\rangle_T = \frac{1}{\sqrt{2\pi}} \int e^{-ikx}\,|\psi_{k,n}\rangle_T \tag{IV.10}$$

Using eqs. (IV.9) one can in fact show that $|\psi_{x,n}\rangle_T$ obeys the equations

$$\hat{Q}|\psi_{x,n}\rangle_T = x\,|\psi_{x,n}\rangle_T$$
$$\hat{P}|\psi_{x,n}\rangle_T = i\,\partial/\partial x\,|\psi_{x,n}\rangle_T \tag{IV.11}$$

One can also relate the states (IV.10) directly to the generator states. Using eq. (II.16) one has

$$|\psi_{x,n}\rangle_T = \frac{1}{\sqrt{2\pi\lambda_n}} \int |\alpha\beta\rangle (\alpha\beta|xn)\, d\alpha\, d\beta \tag{IV.12}$$

where $(\alpha\beta|xn)$ is the Fourier transform of $(\alpha\beta|kn)$

$$\begin{aligned} (\alpha\beta|xn) &= \frac{1}{\sqrt{2\pi}} \int (\alpha\beta|kn)\, e^{-ikx}\, dk \\ &= \frac{e^{-i\beta(x-\alpha)}}{\sqrt{2\pi}}\, \tilde{\phi}_n(x-\alpha) \end{aligned} \tag{IV.13}$$

Here $\tilde{\phi}_n(x)$ is itself the Fourier transform of $\phi_n(k)$.

The states $|\psi_{x,n}\rangle_T$ can be thus written as

$$|\psi_{x,n}\rangle_T = \frac{\hat{\Pi}^{PT}_{x,n}\, |0\rangle}{\sqrt{\lambda_n}}$$

where $\hat{\Pi}^{PT}_{x,n}$ is the Peierls-Thouless double projection operator associated with the operator $\hat{Q}$

$$\hat{\Pi}^{PT}_{x,n} = \int d\alpha\, d\beta\, \frac{e^{-i\beta x}}{2\pi}\, \tilde{\phi}_n(x-\alpha)\, e^{i\beta\hat{Q}}\, e^{-i\alpha\hat{P}}$$

The functions $(\alpha\beta|xn)$ are also eigenfunctions of the overlap kernel $\langle\alpha\beta|\alpha'\beta'\rangle$ with eigenvalue $2\pi\lambda_n$. This is indeed possible due to the degeneracy of the problem (λ_n is independent of k) which implies that any wave packet in k (with fixed n) is also an eigenfunction of the overlap kernel with eigenvalue $2\pi\lambda_n$.

IV.3 - DYNAMICS IN THE GCM COLLECTIVE SUBSPACE

Once a representation in the GCM collective subspace is found, one can imediately write down the restriction of the Hamiltonian to the collective subspace, by just taking matrix elements with respect to the adopted representation. The collective dynamical problem reduces then to the diagonalization of this restricted Hamiltonian.

In the O.P.F. case, the collective wave equation in the momentum representation reads

$$\int dk'\, h(k,k')\, \varphi(k',t) = i\hbar \frac{\partial \varphi(k,t)}{\partial t} \qquad \text{(IV.14)}$$

where

$$\begin{aligned} h(k,k') &= {}_{\gamma}\langle \Psi_k | \hat{H} | \Psi_{k'} \rangle_{\gamma} \\ &= \int \frac{d\alpha\, d\alpha'}{2\pi} \frac{(k|\alpha)}{\sqrt{\Lambda(k)}} \langle \alpha | \hat{H} | \alpha' \rangle \frac{(\alpha'|k')}{\sqrt{\Lambda(k')}} \end{aligned} \qquad \text{(IV.15)}$$

and

$$\varphi(k,t) = {}_{\gamma}\langle \Psi_k | \varphi(t) \rangle$$

with

$$\hat{S}_1 | \varphi(t) \rangle = | \varphi(t) \rangle$$

The matrix elements of any other operator $\hat{A}$ between states defined in S_1 can also be written in terms of a matrix $A(k,k')$ which is given by an expression analogous to eq. (IV.15) where in place of $\hat{H}$ one has the operator $\hat{A}$.

We can also try and express any operator defined in S_1 (or the restriction of any operator to the collective subspace S_1) in terms of the "fundamental" dynamical variables $\hat{Q}_1$ and $\hat{P}_1$. Considering the Hamiltonian as an example one has[10]

$$\hat{S}_1 \hat{H} \hat{S}_1 = \sum_{\substack{m=0 \\ m \text{ even}}}^{\infty} \frac{1}{2^m} \hat{P}_1^{(m)} \{ \hat{H}^{(m)}(\hat{Q}_1) \} \tag{IV.16}$$

where $\hat{A}^{(m)}\{\hat{B}\}$ is the mth anti-commutator of $\hat{A}$ and $\hat{B}$

$$\hat{A}^{(m)}\{\hat{B}\} = \underbrace{\{\hat{A}, \{\hat{A}, \cdots \{\hat{A}, \hat{B}\} \cdots \}\}}_{m \text{ anticommutators}}$$

and $\hat{H}^{(m)}(\hat{Q}_1)$ is

$$\hat{H}^{(m)}(\hat{Q}_1) = \int dx \frac{(-ix)^m}{m!} \langle \Psi_{Q_1+\frac{x}{2}} | \hat{H} | \Psi_{Q_1-\frac{x}{2}} \rangle$$

$$= \int \frac{dk}{m!} e^{ikQ_1} \frac{d^m}{dk^m} \langle \Psi_{K+k/2} | \hat{H} | \Psi_{K-k/2} \rangle \Big|_{K=0} \tag{IV.17}$$

In the case of the T.C.P.F. the wave equation in the collective subspace is

$$\sum_{\mu'} \int dk' \, h_{\mu\mu'}(k,k') \varphi_{\mu'}(k',t) = i\hbar \frac{\partial \varphi_\mu(k,t)}{\partial t} \tag{IV.18}$$

where

$$h_{n,n'}(k,k') = {}_T\langle \psi_{k,n} | \hat{H} | \psi_{k',n'} \rangle_T$$

$$= \int \frac{d\alpha\, d\beta\, d\alpha'\, d\beta'}{2\pi} \frac{(k\, n|\alpha\beta)}{\sqrt{\lambda_n}} \langle \alpha\beta | \hat{H} | \alpha'\beta' \rangle \frac{(\alpha'\beta'|k',n')}{\sqrt{\lambda_{n'}}} \qquad \text{(IV.19)}$$

and

$$\varphi_n(k,t) = {}_T\langle \psi_{k,n} | \varphi(t) \rangle$$

We can also write the matrix elements of any operator between states in S_2 in terms of the matrix elements of this operator in the base representation $|\psi_{k,n}\rangle_T$.

V - THE SEPARATION OF COLLECTIVE AND INTRINSIC DEGREES OF FREEDOM

The construction of the OPF and of the TCPF in the preceding sections was based on the consideration of a canonically conjugated pair of collective operators, $\hat{Q}$ and $\hat{P}$, defined in the full many-body Hilbert space. We may thus consider a canonical transformation, e.g. from microscopic coordinates and momenta, to a new set of operators that includes the collective operators $\hat{Q}$ and $\hat{P}$. Considering, together with $\hat{Q}$, the remaining N-1 coordinate operators

$$\{\hat{\xi}\} \equiv (\hat{\xi}_1, \hat{\xi}_2 \cdots \hat{\xi}_{N-1})$$

which, by the canonical nature of the transformation must commute with both $\hat{Q}$ and $\hat{P}$, we can arrive at a coordinate representation of the full many-body space defined by the kets

$$|Q, \xi\rangle$$

chosen as eigenkets of $\hat{Q}$ and of the operators $\hat{\xi}$. This representation is actually a product representation in the sense that we can write

$$|Q, \xi\rangle = |Q\rangle \otimes |\xi\rangle$$

where the $|Q\rangle$ span a Hilbert space for one single degree of freedom, the collective space, and the $|\xi\rangle$ are likewise associated with a Hilbert space for N-1 degrees of freedom, the intrinsic space. In what follows we shall make a formal use of this representation of the full many-body Hilbert space in order to exhibit the factorization properties of the GCM collective subspaces S_1 and S_2, constructed in terms of the OPF and of the TCPF of generator states respectively. We shall refer to Q and to ξ as the collective coordinate and the intrinsic coordinates respectively. Unless otherwise stated, we understand them as a representation of the full many-body space. It should be always kept in mind, moreover that both S_1 and S_2 carry all the N degrees of freedom of the many-body system under consideration. They are distinguished from the full many-body space in that they contain various imposed correlations among the N degrees of freedom. The following discussion will be aimed precisely at exposing the general nature of these correlations in each of the two cases.

We begin by considering the wavefunctions associated by the representation $|Q\xi\rangle$ with the TCPF base vectors. These are easily found to be

$$\langle Q,\xi|\Psi_{k,n}\rangle_T = \frac{e^{ikQ}}{\sqrt{2\pi}}\ \chi_n(\xi) \tag{V.1}$$

where the orthonormal states $\{\chi_n\}$, which depend only on the intrinsic coordinates, are given by

$$\chi_n(\xi) = \frac{1}{\sqrt{\lambda_n}}\int \tilde{\phi}_n(Q)\,\langle Q\,\xi|0\rangle\, dQ \tag{V.2}$$

The functions $\tilde{\phi}_n(Q)$ are the Fourier transforms of the $\phi_n(k)$ (see eq. (II.12)). Using our previous results, it follows that the number of orthonormal states χ_n is equal to the number of eigenvectors of the reduced kernel (II.11) with non-vanishing eigenvalues. We see now that they span a subspace of the intrinsic space associated with the N-1 degrees of freedom $\hat{\xi}$. Furthermore, using eq. (III-2) the reference state $|0\rangle$ can be naturally expressed in terms of the $\chi_n(\xi)$ as

$$\langle Q\xi|0\rangle = \sum_{m,\lambda_m\neq 0} \sqrt{\lambda_m}\ \tilde{\phi}_m(Q)\ \chi_m(\xi) \tag{V.3}$$

The states $|\psi_{k,n}\rangle_T$, eq. (V.1), thus come out as products of a collective wave function (a plane wave in the collective variable) and an intrinsic wave function (depending on the intrinsic variables ξ alone); and this is true even when the reference state $|0\rangle$ does not factor in the representation $|Q\xi\rangle$.

The states $|\psi_k\rangle_Y$, on the other hand, which are a base in the subspace generated by the O.P.F. of generator states are associated by the $|Q\xi\rangle$ representation with the wave functions

$$\langle Q\xi|\Psi_h\rangle_Y = \frac{1}{\sqrt{2\pi}}\ e^{ihQ}\ X_h(\xi) \tag{V.4}$$

where

$$\begin{aligned} X_h(\xi) &= \frac{1}{\sqrt{2\pi\Lambda(h)}} \int dQ\ e^{-ihQ}\langle Q\xi|0\rangle \\ &= \sum_{m,\lambda_m\neq 0} V_m(h)\, X_m(\xi) \end{aligned} \tag{V.5}$$

These wave functions appear as the product of a collective wave function and an intrinsic wave function which, however, depends on the eigenvalue k of the operator $\hat{P}$. Consequently the states $|\psi_k\rangle_Y$ factor into independent collective and intrinsic parts only when the reduced kernel (II.11) has only one non-vanishing eigenvalue. In this case, in fact, the reference state $|0\rangle$ itself admits a similar factorization i.e. (see eqs. (V.3) and (A.5))

$$\langle Q\xi|0\rangle = \tilde{\phi}_0(Q)\,\chi_0(\xi) \tag{V.6}$$

and by eqs. (V.5) and (III.8) one has

$$\chi_k(\xi) = \chi_0(\xi)$$

When such a particular reference state is used to generate the TCPF, moreover, one finds that the states $|\psi_k\rangle_Y$ are equal to the states $|\psi_{k,o}\rangle_T$ and the subspaces S_1 and S_2 become identical.

It follows from these properties that the natural representation $|\psi_{k,n}\rangle_T$ for the subspace S_2 generated by the TCPF is itself a product representation. In fact S_2 appears as the direct product of the collective space $\mathcal{H}_c$ with an intrinsic subspace spanned by the wave functions $\chi_n(\xi)$. The dimensionality of this intrinsic subspace is given by the number of eigenvectors of the reduced kernel (II.11) with non-vanishing eigenvalues. This product decomposition of S_2 holds for an arbitrary reference state $|o\rangle$. For reasons to be made clear below, we refer to this factorization property as the Galilean invariance of the GCM collective subspace. On the other hand, the nature of the natural representation $|\psi_k\rangle_Y$ for the subspace S_1 shows that in general S , is not decomposable onto collective and intrinsic parts (i.e., it is not Galilean invariant). In the special case when the reference state $|o\rangle$ itself factors in a product of an intrinsic wave function and a collective wave function, however, the GCM subspace S_1 , which in this case is identical to the subspace S_2 , is in fact Galilean invariant. It is given by the direct product of the collective space $\mathcal{H}_c$ and a one-dimensional subspace of the intrinsic space.

To discuss the properties of the restricted dynamics of the GC scheme consider first the concept of an ideal collective subspace which was discussed throughly in Chapter I. The ideal collective subspace $\hat{S}_c$ is equal to the product of the collective space $\mathcal{H}_c$ and a one-dimensional subspace of the intrinsic space $|I\rangle$, such that

$$[\hat{S}_c, \hat{H}] = 0 \tag{V.7}$$

Eq. (V.7) shows that there is no coupling between intrinsic and collective degrees of freedom in $\hat{S}_c$, and that the spectrum of $\hat{S}_c\hat{H}\hat{S}_c$ which in what follows we will call the "collective spectrum", reproduces part of the exact energy spectrum of $\hat{H}$. The "non-collective spectrum" which is described by the restricted hamiltonian $\hat{R}_c\hat{H}\hat{P}_c$, where $\hat{R}_c$ is the complementary projection operator

$$\hat{R}_c = \hat{1} - \hat{S}_c$$

is in this case completely decoupled from the "collective" one. The GCM collective hamiltonian $\hat{S}_2\hat{H}\hat{S}_2$ will thus have all the properties of $\hat{S}_c\hat{H}\hat{S}_c$ provided the ideal intrinsic state $|I\rangle$ be a vector defined in the GCM intrinsic space spanned by the states $\{\chi_n\}$. The presence of more than one intrinsic mode in S_2 will cause the GCM hamiltonian $\hat{S}_2\hat{H}\hat{S}_2$ to have, besides the "collective" spectrum, a "non-collective" spectrum completely decoupled from the "collective" one. On the other hand had we considered the GCM collective subspace S_1 , which in general does not factor into a product space, we would find that as a result of the "kinematical coupling" between the "collective" and "non- collective" states (see eqs. (V.5) and (V.11)) its spectrum has a "hybrid" character and can differ considerably from the exact "collective" spectrum.

A simple illustration of these facts is provided by the translation of a Galilean invariant system. Here the hamiltonian is

$$\hat{H} = \hat{H}_c + \hat{H}_I$$

The collective hamiltonian $\hat{H}_c$ is just

$$\hat{H}_c = \frac{\hat{P}^2}{2M} \quad , \quad M = Am \tag{V.8}$$

and we set up GC schemes using $\hat{P}$ and the conjugate center of mass position operator $\hat{Q}$ as collective variables. As discussed above, when the Q-dependence of the reference state factors the GCM collective subspaces S_1 and S_2 (corresponding to the OPF and to the TCPF respectively) coincide and the GCM collective hamiltonian becomes

$$h(k,k') = \left(\frac{k^2}{2M} + \langle \chi_0 | \hat{H}_I | \chi_0 \rangle\right) \delta(k-k') \tag{V.9}$$

We see that the description of the translational motion is exact and this fact stems from the Galilean invariance of the collective subspace. However, even in the case when the reference state does not factor in a product wave function, the collective subspace generated by the T.C.P.F. is still Galilean invariant and the projected hamiltonian is

$$h_{m,m'}(k,k') = \left(\frac{k^2}{2M} \delta_{mm'} + \langle \chi_m | H_I | \chi_{m'} \rangle\right) \delta(k-k') \tag{V.10}$$

Thus we see that the description of the translational motion is exact, whereas the intrinsic states are approximated by the diagonalization of $\hat{H}_I$ in the subspace spanned by the orthonormal states $\{\chi_n\}$. In the O.P.F. case, S_1 is not Galilean invariant and the projected hamiltonian is

$$h(k,k') = \delta(k-k')\left(\frac{k^2}{2M} + \sum_{n,n'} V_n^*(k)\langle\chi_n|\hat{H}_I|\chi_{n'}\rangle V_{n'}(k)\right) \quad (V.11)$$

As a result of the kinematical coupling, the translational mass, defined in terms of the coefficient of k^2, comes out wrong in the above equation.

This discussion shows clearly that this defect is not to be ascribed to the generator coordinate method itself, but rather to the bad choice of the generator states. A good choice should give rise to a Galilean invariant collective subspace. This requirement is always satisfyed by the T.C.P.F..

VI - APPLICATIONS

VI.1 - GIANT RESSONANCES AND SUM RULES

Extensive calculations of the properties of the giant ressonances in light nuclei were performed by Flocard and Vautherin[5], in the framework of the generator coordinate method. Taking these very complete calculations as an example, we illustrate the qualitative understanding of the content of a GCM calculation that can be gained using the ideas developed in this paper.

a) Isoscalar quadrupole and monopole oscillations

Nuclear collective monopole and quadrupole oscillations are described in reference 5 in terms of a family of Slater determinants of harmonic oscillator wave functions, where the size parameter of the oscillator in the z-direction, γ_z,

$$\gamma_z = \frac{m\omega_z}{\hbar}$$

and the size parameter in the plane perpendicular to the z-direction

$$\gamma_\perp = \frac{m\omega_x}{\hbar} = \frac{m\omega_y}{\hbar}$$

are treated as generator coordinates. These generator states can be written as

$$|\gamma_z,\gamma_\perp\rangle = e^{i\left(\ln\sqrt{\gamma_z/\gamma_0}\,\hat{D}_3 + \ln\sqrt{\gamma_\perp/\gamma_0}\,(\hat{D}_1+\hat{D}_2)\right)}|0\rangle \quad \text{(VI.1.1)}$$

where $\hat{D}_i$ is a dilatation operator in the i-direction

$$\hat{D}_i = \sum_{j=1}^{A} \frac{\hat{x}_i(j)\,\hat{p}_i(j) + \hat{p}_i(j)\,\hat{x}_i(j)}{2} \qquad i = 1,2,3 \tag{VI-1.2}$$

and the reference state $|0\rangle$ is a Slater determinant of harmonic oscillator wave functions for which the size parameter has the equilibrium value γ_0 .

It has been shown in reference 1 that the collective subspace is invariant by a change of labels of the generator states. Here we use this freedom to rewrite eq. (VI.1.1) in terms of new generator coordinates α_1 and α_2 defined by

$$\frac{\gamma_z}{\gamma_0} = e^{2\alpha_1}$$

$$\frac{\gamma_\perp}{\gamma_0} = e^{2\alpha_2}$$

in terms of which

$$|\gamma_z\gamma_\perp\rangle \to |\alpha_1\alpha_2\rangle = e^{i(\alpha_1\hat{D}_3 + \alpha_2(\hat{D}_1+\hat{D}_2))}\,|0\rangle \tag{VI.1.3}$$

As $\hat{D}_3$ and $\hat{D}_1 + \hat{D}_2$ are commuting operators, the above states are a trivial generalization of a standard O.P.F. and so all the properties previously discussed hold.

Nuclear monopole oscillations are described in reference 5 by isotropic oscillators given by

$$|\alpha\rangle = |\alpha_1 = \alpha, \alpha_2 = \alpha\rangle = e^{i\alpha\hat{D}}\,|0\rangle \tag{VI.I.4}$$

where $\hat{D}$ is the dilatation operator

$$\hat{D} = \sum_{i=1}^{3} \hat{D}_i$$

There is a representation in the collective subspace S_1^o, associated with the generator states $|\alpha\rangle$, in which $\hat{D}$ is diagonal. The base vectors defining this representation are the normalized Peierls-Yoccoz projections of the reference state $|o\rangle$, associated with the dilatation operator $\hat{D}$. Although an operator canonically conjugated to the dilatation operator $\hat{D}$ in the full Hilbert space, is not given, we can find, using eqs. (IV.1), an operator conjugated to $\hat{D}$ in the collective subspace S_1^o.

Nuclear quadrupole oscillations are described by the anisotropic oscillators (VI.1.3), in which we impose the volume conservation condition

$$\gamma_\perp^2 \gamma_z = \gamma_0^3$$

which in terms of α_1 and α_2 yields

$$\alpha_2 = -\frac{\alpha_1}{2}$$

The generator states $|\alpha_1\ \alpha_2\rangle$ eq. (VI.1.3), becomes, using this condition,

$$\begin{aligned} |\alpha\rangle &= |\alpha_1 = -2\alpha, \alpha_2 = \alpha\rangle \\ &= e^{i\alpha(\hat{D}_1 + \hat{D}_2 - 2\hat{D}_3)} |0\rangle \end{aligned} \qquad \text{(VI.1.5)}$$

Again these generator states are a standard O.P.F. and there is a representation in the collective subspace S_1^2, associated with the generator states $|\alpha\rangle$ in which $\hat{D}_Q$,

$$\hat{D}_Q = \hat{D}_1 + \hat{D}_2 - 2\hat{D}_3$$

is diagonal

The case of coupled isoscalar monopole and quadrupole oscillations are described by the generator states (VI.1.3). Thus, there is a representation in the collective subspace $S_1^{0,2}$ associated with the generator states $|\alpha_1,\alpha_2\rangle$, in which the commuting operators $\hat{D}_1$ and $\hat{D}_1+\hat{D}_3$ are diagonal.

b) Dipole oscillations

The generator states are in this case chosen as

$$|\alpha\rangle = e^{-i\alpha\hat{P}_3}|0\rangle \qquad \text{(VI.1.6)}$$

where $\hat{P}_3$ is the z-component of the relative momentum between protons and neutrons, which for self-conjugate nuclei is

$$\begin{aligned} \hat{\vec{P}} &= \frac{1}{2}(\hat{\vec{P}}_Z - \hat{\vec{P}}_N) \\ \hat{\vec{P}}_Z &= \sum_{i=1}^{A} \hat{\vec{p}}(i)\frac{(1+\tau_3(i))}{2} \\ \hat{\vec{P}}_N &= \sum_{i=1}^{A} \hat{\vec{p}}(i)\frac{(1-\tau_3(i))}{2} \end{aligned} \qquad \text{(VI.1.7)}$$

In this case the operator which is canonical to $\hat{P}$ is immediately given as

$$\hat{\vec{Q}} = \hat{\vec{R}}_Z - \hat{\vec{R}}_N \qquad \text{(VI.1.8)}$$

Thus the dipole oscillations can be described by the states $|\alpha\rangle$ which are standard O.P.F., as is done in reference 5, or by the generator states $|\alpha\beta\rangle$

$$|\alpha,\beta\rangle = e^{-i\alpha\hat{P}_3}\, e^{i\beta\hat{Q}_3}\,|0\rangle \qquad \text{(VI.1.9)}$$

which are a standard T.C.P.F..

For the popular choice which consists in taking for the reference (fiducial) state $|o\rangle$ a double closed shell Slater determinant of harmonic oscillator wave functions, one immediately sees that it is the vacuum of the boson operator

$$\hat{b} = \frac{1}{\sqrt{2}}\left(\frac{\hat{Q}_3}{b_0} + i\,\hat{P}_3 b_0\right) \qquad \text{(VI.1.10)}$$

where

$$b_0 = \sqrt{\frac{4\hbar}{Am\omega_0}}$$

This fact shows that the T.C.P.F. (V.1.9) is locally redundant in the sense of reference 8 and as discussed in section V, implies the factorization of the reference state $|o\rangle$. The consequence of all this is that the collective subspaces associated with each of the families of generator states are identical. Furthermore one can find a representation in the collective subspace in which $\hat{Q}_3$ or $\hat{P}_3$ are diagonal.

Although the discussion had up to this point only a kinematical character, one can treat the dynamics, following the ideas of section IV.3. Once one has a representation in the GCM collective subspace one can construct the GCM collective hamiltonian and find its spectrum. This actually has been done for monopole[11] and dipole oscillations[12].

c) Sum rules

In the case of sum rules the important question is to investigate under what conditions the sum rule is exhausted in the GCM collective subspace.

For ease of presentation consider the positive sum rules m_1 and m_3 which are given by

$$m_1 = \frac{1}{2} \langle \Psi_0 | [\hat{A}, [\hat{H}, \hat{A}]] | \Psi_0 \rangle \tag{VI.1.11}$$

$$m_3 = \frac{1}{2} \langle \Psi_0 | [\hat{A}, [\hat{H}, [\hat{H}, [\hat{H}, \hat{A}]]]] | \Psi_0 \rangle \tag{VI.1.12}$$

These sum rules will be exhausted in the GCM collective subspace, provided one has[5]

$$\begin{aligned} m_1^{(s)} &= \frac{1}{2} \langle \Psi_0^{(s)} | [\hat{A}, [\hat{H}_{ss}, \hat{A}]] | \Psi_0^{(s)} \rangle \\ &= \frac{1}{2} \langle \Psi_0^{(s)} | [\hat{A}, [\hat{H}, \hat{A}]] | \Psi_0^{(s)} \rangle \end{aligned} \tag{VI.1.13}$$

$$\begin{aligned} m_3^{(s)} &= \frac{1}{2} \langle \Psi_0^{(s)} | [\hat{A}, [\hat{H}_{ss}, [\hat{H}_{ss}, [\hat{H}_{ss}, \hat{A}]]]] | \Psi_0^{(s)} \rangle \\ &= \frac{1}{2} \langle \Psi_0^{(s)} | [\hat{A}, [\hat{H}, [\hat{H}, [\hat{H}, \hat{A}]]]] | \Psi_0^{(s)} \rangle \end{aligned} \tag{VI.1.14}$$

It can be easily shown that for m_1 it is sufficient that

$$[\hat{S}, \hat{A}] = 0 \tag{VI.1.15}$$

and for m_3 one must have in addition to (VI.1.15) also

$$[\hat{S}, [\hat{H}, \hat{A}]] = 0$$

According to reference 5 (equation C.3) one has

$$[S_1^0, \hat{r}^2] = 0$$

$$[S_1^2, \hat{Q}] = 0$$

where $\hat{r}^2$ and $\hat{Q}$ are the square radius and quadrupole moment respectively

$$\hat{r}^2 = \sum_{i=1}^{A} \hat{r}^2(i)$$

$$\hat{Q} = \sum_{i=1}^{A} \left(x(i)^2 + y(i)^2 - 2\, z(i)^2 \right)$$

Assuming a local two-body interaction (except for possible spin and isospin exchange terms) one has[13,14]

$$[\hat{H}, \hat{r}^2] = [\hat{T}, \hat{r}^2] = -\frac{2i}{m} \hat{D}$$

$$[\hat{H}, \hat{Q}] = [\hat{T}, \hat{Q}] = -\frac{2i}{m} \hat{D}_Q$$

which gives

$$[S_1^0, [\hat{H}, \hat{r}^2]] = 0$$

$$[S_1^2, [\hat{H}, \hat{Q}]] = 0$$

thus showing that m_1 and m_3 are completely exhausted in the respective collective subspaces S_1^o and S_1^2 .

VI.2 - SCATTERING: "CLUSTER" STATES AND THE PROPER DEFINITION OF CHANNEL STATES

From a rather formal point of view, one may quite generally associate a possible continuous part of the spectrum of the collective hamiltonian $\mathcal{S}\mathcal{H}\mathcal{S}$ for a finite system to scattering processes that survived the truncation of the original Hilbert space by means of the projector $\hat{S}$. In order to discuss the possible significance of this scattering, however, it is essential to have at least an adequate understanding of the allowed asymptotically free states or channels. We shall see below how the procedures we discuss for the construction of collective spaces can be naturally brought to bear on this matter. The main point is that properly defined channels must sustain a twofold Galilean invariance, namely, invariance under translations and boosts of the overall center of mass and asymptotic invariance under changes of relative distance and (asymptotic) relative momentum. In current applications of the GCM to scattering problems these conditions are met by requiring adequate factorization properties of the many-body generator states[15]. Many of the developed techniques, however, are based directly on the consideration of the GCM equation, rather than a Schrodinger equation based on a suitably constructed collective Hamiltonian[16,17]. The use of Peierls-Yoccoz collective spaces is sufficient to construct a collective Hamiltonian when the factorization properties of the generator states are adequate. More general cases can in principle also be handled, however, through the consideration of Peierls-Thouless type collective spaces.

A more delicate problem in the GCM treatment of scattering problems concerns the nature of the interactions allowed after truncation of the many-body phase space, in relation to the dynamical behavior of the unrestricted system. This cannot in general be decided in terms of the simple arguments developed here.

We will for definiteness develop the discussion around the consideration of many-body states which are written as the (suitably antisymmetrized) product of localized cluster states displaced relatively to each other. States of this kind are extensively used to study the structure of light nuclei, for instance[18], in addition to their obvious appeal for GCM treatments of collision problems involving the systems suposedly well represented by the considered clusters. In order to keep the resulting collective dynamics as simple as possible, we restrict ourselves moreover to the case of cluster pairs only. Using the notation $\vec{\alpha}_i$ (i=1,2) for the cluster positions (to be taken as generator coordinates), and the collective symbols x_i for the set of particle coordinates in each cluster, we thus consider states of the type

$$\Phi(x_1\vec{\alpha}_1; x_2\vec{\alpha}_2) = \mathcal{A}\left[\varphi_1(x_1;\vec{\alpha}_1)\,\varphi_2(x_2;\vec{\alpha}_2)\right]$$

Due to the overall Galilean invariance of the total hamiltonian $\hat{H}$ it is useful to introduce mean position and relative generator coordinates $\vec{A}$ and $\vec{\alpha}$ defined as

$$\vec{A} = \frac{M_1\vec{\alpha}_1 + M_2\vec{\alpha}_2}{M_1 + M_2} \qquad \text{and} \qquad \vec{\alpha} = \vec{\alpha}_1 - \vec{\alpha}_2$$

M_1 and M_2 being the masses of the two clusters. Now

$$\Phi(x_1\vec{\alpha}_1, x_2\vec{\alpha}_2) \to \Phi(x_1 x_2, \vec{A}\vec{\alpha}) = \mathcal{A}\left[\varphi_1(x_1;\vec{A}+\frac{M_2\vec{\alpha}}{M_1+M_2})\,\varphi_2(x_2,\vec{A}-\frac{M_1\vec{\alpha}}{M_1+M_2})\right]$$

wich can also be written in terms of the cluster momentum operators P_i as

$$\Phi(x_1x_2;\vec{A}\vec{\alpha}) = \mathcal{A}\left[e^{-i(\vec{A}+\frac{M_2}{M_1+M_2}\vec{\alpha})\cdot\vec{P}_1}\varphi_1(x_1,0)\,e^{-i(\vec{A}-\frac{M_1}{M_1+M_2}\vec{\alpha})\cdot\hat{\vec{P}}_2}\varphi_2(x_2,0)\right] \tag{VI.2.1}$$

$$= e^{-i\vec{A}\cdot\vec{P}}\mathcal{A}\left[e^{-i\vec{\alpha}\cdot\vec{p}}\varphi_1(x_1,0)\varphi_2(x_2,0)\right]$$

where total and relative momenta have been introduced as

$$\vec{P} = \vec{P}_1 + \vec{P}_2 \qquad \vec{p} = \frac{M_2}{M_1+M_2}\vec{P}_1 - \frac{M_1}{M_1+M_2}\vec{P}_2$$

Since $\vec{A}.\vec{P}$ is a symmetric operator, the corresponding exponential can be taken out of the antisymmetrizer brackets.

The generator states (VI.2.1) have thus quite generally very simple overlap properties with respect to the mean position generator coordinate $\vec{A}$. In fact their form alone guarantees that the overlap kernel will be a function of the difference $\vec{A}-\vec{A}'$ only. The dependence of the overlap kernel on $\vec{\alpha}$ and $\vec{\alpha}'$ is however more complicated. This come about due to the effects of the antisymmetrization, and is related to Pauli blocking effects at finite cluster separations. For asymptotically large values of $|\vec{\alpha}|$ and $|\vec{\alpha}'|$, in fact, only direct (as opposed to exchange) terms survive, and the overlap kernel retains a dependence on $\vec{\alpha} - \vec{\alpha}'$ only. We may thus write

$$\langle \Phi(\vec{A},\vec{\alpha}) | \Phi(\vec{A}',\vec{\alpha}')\rangle = N_\infty(\vec{A}-\vec{A}', \vec{\alpha}-\vec{\alpha}') - N_{exch}(\vec{A}-\vec{A}', \vec{\alpha}, \vec{\alpha}')$$

where N_{exch} is a short-range kernel (i.e., vanishing in the asymptotic region). The effects of this short-range kernel are of course of fundamental importance for the description of the scattering, although, by its essential short-range character, they do not influence the <u>asymptotic</u> structure of the channels. Since we focus on this latter property, we are justified in neglecting N_{exch} here. Once the asymptotic nature of the channels is established, exchange effects can always be handled, in principle, using tools which have been repeatedly discussed in the literature[19], or by just considering suitable energy-dependent non-local effective potentials as done in the Resonating Group Method or in earlier applications of the GCM to scattering problems[16].

We concern ourselves thus with the simpler set of generator states

$$\Phi_\infty(x_1,x_2;\vec{A}\vec{\alpha}) = e^{-i\vec{A}.\vec{P}}\, e^{-i\vec{\alpha}.\vec{p}}\, \varphi_1(x_1,0)\, \varphi_2(x_2,0)$$

Noting that they are a Peierls-Yoccoz family with respect both to mean position and to relative position of the two clusters, it is immediately clear that they will generate a subspace with the two required types of Galilean invariance only in the special case where the cluster product factorizes into a Center of Mass function times a function of the separation between the centers of mass of the two clusters and a single "intrinsic" wave function for the two clusters. This double factorization has actually been required in practical calculations done so far with the GCM[15,16,18].

To deal with less well behaved cluster product states one can fix the desired properties of the collective subspace by enlarging the generator family so as to include boosted states like

$$\Phi_{\infty}(x_1,x_2,\vec{A}\,\vec{B}\,\vec{\alpha}\,\vec{\beta}) = e^{-i\vec{A}\cdot\vec{P}}\, e^{i\vec{B}\cdot\vec{Q}}\, e^{-i\vec{\alpha}\cdot\vec{p}}\, e^{i\vec{\beta}\cdot\vec{q}}\, \varphi_1(x_1,0)\,\varphi_2(x_2,0) \qquad \text{(VI.2.2)}$$

where now $\vec{Q}$ is the center of mass position operator canonically conjugate do $\vec{P}$ and a similar relation holds between $\vec{q}$ and the relative momentum $\vec{p}$. Again the overlap of these non-antisymmetrized states differs from the full overlap kernel by short-range exchange terms only.

One can now in a straithforward way apply the TCPF procedure given in section II.2 to the states (VI.2.2) to obtain the orthonormal basis for the collective space

$$\langle x_1 x_2 | \Psi_{\vec{K}\vec{k}m} \rangle = \frac{1}{\sqrt{\lambda_m}}\, \hat{\Pi}^{PT}_{\vec{K}\vec{k}m}\, \varphi_1(x_1,0)\,\varphi_2(x_2,0) \qquad (\lambda_m \neq 0) \qquad \text{(VI.2.3)}$$

with the doubly Peierls-Thouless projector $\hat{\Pi}$ given here as

$$\hat{\Pi}^{PT}_{\vec{k},\vec{K},n} = \int d\vec{\alpha}\, d\vec{\beta} \int d\vec{A}\, d\vec{B}\; \frac{e^{i\vec{k}\cdot\vec{\alpha}}}{2\pi} \frac{e^{i\vec{K}\cdot\vec{A}}}{2\pi} \phi_n(\vec{\beta}-\vec{k}, \vec{B}-\vec{K}) \; \times$$

$$\times\; e^{-i\vec{\alpha}\cdot\vec{p}}\, e^{i\vec{\beta}\cdot\vec{q}}\, e^{-i\vec{A}\cdot\vec{P}}\, e^{i\vec{B}\cdot\vec{Q}}$$

The function $\phi_n(\vec{\beta},\vec{B})$ is chosen as an eigenfunction of the reduced kernel

$$\langle \vec{\beta}\,\vec{B} | \hat{n} | \vec{\beta}'\,\vec{B}' \rangle = \langle \varphi_1 \varphi_2 | e^{-i\vec{\beta}\cdot\vec{q}}\, \delta(\vec{p})\, e^{i\vec{\beta}'\cdot\vec{q}}\, e^{-i\vec{B}\cdot\vec{Q}}\, \delta(\vec{P})\, e^{i\vec{B}'\cdot\vec{Q}} | \varphi_1 \varphi_2 \rangle$$

with eigenvalue λ_n (cf. eqs. (II.11) and (II.12)). We see thus that by means of Peierls-Thouless projections we obtain in general several (asymptotically) orthogonal channels labeled by the index n, from a single cluster product. They correspond to subspaces of the collective space having the proper decoupling of different orthogonal, intrinsic states associated with the ϕ_n. Whenever the special factorization properties stated above apply, only one of the eigenvalues λ_n will fail to vanish, and one recovers the subspace that can in this case be also obtained from the OPF and Peierls-Yoccoz projections. The factorization e.g. of the overall center of mass dependence of the cluster product, on the other hand, implies the factorization of the B,B' dependence of the reduced kernel. In this case the extra generator coordinate B does not enlarge the collective subspace and different channels ϕ_n become associated with the coordinate $\vec{\beta}$ only.

We see in conclusion that the collective hamiltonians obtained from the GCM can be used directly to discuss scattering situations, subject to the usual warnings concerning the significance of the retained collective degrees of freedom. The advantage in their use, rather than the use of procedures based directly on the consideration of the corresponding Griffin-Hill-Wheeler equations[15] hinges probably on the asymptotic information being expressed immediately in familiar language and on the avoidance of the unpleasant kinematically generated instabilities usually present in direct solutions of the GHW equation. It is probably also worth stressing that the consideration of vector generator coordinates leads to a rotation-invariant collective subspace. The angular momentum analysis of the collective scattering problem can thus be obtained with familiar partial-wave decomposition techniques applied to the dynamical problem defined by the collective hamiltonian.

VII - CONCLUDING REMARKS

The application of the GCM to the dynamics of a quantum many-body system amounts to consider the truncated problem that one obtains by restricting the system to a complete subspace of the many-body Hilbert space. In the preceding sections we discussed properties of the subspaces associated with a class of generator states of frequent usage, namely generator states obtained by applying generalized translations (and boosts) to a given reference state. The use of such a family in fact implies a decision, which has a strong dynamical content, in favor of some collective dynamical variable (and its canonically conjugate pair) as the relevant one. A clear and trivial example is the use of the total momentum (and the center-of-mass position) to describe translations. A less trivial and well exploited case is the use of dilatation operators to generate nuclear shape vibrations[5,11].

Using tools developed earlier[1,2] we examine in detail the properties of the subspaces generated by one (eq. (II.1)) and two conjugate parameter (eq, (II.7)) families of generator states. It may be noted that the construction of these families involves only the one-parameter unitary groups having the chosen collective dynamical variables as generators. This guarantees that the extention of the discussion to cases in which these groups exist while the corresponding generators are rather awkward objects (such as rotations) is in principle straightforward. In fact, it merely involves the consideration of a Weyl system instead of the canonical pair of Generators.

Orthonormal bases in the GCM collective subspaces can be constructed naturally in terms of Peierls-Yoccoz and Peierls-Thouless projections of the reference state, respectively in the case of the one- and two-parameter families. In the latter case, we show that the GCM collective subspace is always an eigenspace of each of the canonical generators (i.e., they both commute with the projection onto the GCM collective subspace). The same is in general not true for the space constructed from the one-parameter family, which is in general an eigenspace of one of the generators only. We also show explicitely, however, that the two types of GCM collective subspace actually do coincide when the reference state involved in the construction of the family of generator states has special factorization properties. The two-parameter family becomes in this case "redundant"(8,9), a fact which can be exploited e.g. in terms of the existence of well-behaved "continuous representations" in the sense of ref. 7 (see also ref. 17).

The truncated dynamics is ruled by the GCM collective Hamiltonian which is defined as the restriction of the many-body Hamiltonian to the GCM collective subspace. When the GCM collective subspace is not an eigenspace of the two members of the chosen canonical pair of collective generators, we show that the GCM collective Hamiltonian contains spurious (i.e., kinematically generated) couplings btween the corresponding collective variables and other , "intrinsic" variables. This effect is responsible e.g. for the incorrect translational mass that one in general obtains by means of Peierls-Yoccoz projections. The use of GCM collective subspace generated from two conjugate parameter families completely avoids this difficult.

We believe that a through explicitation of these results considerably improves the qualitative understanding that one has of the content of existing GCM calculations such as those of ref. 5. Also the definition of appropriate asymptotic states in current GCM descriptions of scattering situations(15,18) is considerably enlightned by them. In fact, in both cases the use of families of generator states of the kind considered here is widespread.

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APPENDIX A

The eigenfunctions and eigenvalues of the semi-positive definite hermitian kernel

$$(\alpha\beta|\hat{N}|\alpha'\beta') = \langle\alpha\beta|\alpha'\beta'\rangle$$
$$= \langle 0|\, e^{-i\beta\hat{Q}}\, e^{i(\alpha-\alpha')\hat{P}}\, e^{i\beta'\hat{Q}}\, |0\rangle \tag{A.1}$$

are determined by the equation

$$\int (\alpha\beta|\hat{N}|\alpha'\beta')(\alpha'\beta'|hm)\, d\alpha' d\beta' = 2\pi\lambda_m(h)\,(\alpha\beta|hm) \tag{A.2}$$

Inserting the ansatz

$$(\alpha\beta|hm) = \frac{e^{ih\alpha}}{\sqrt{2\pi}}\;\phi_{h,m}(\beta)$$

into equation (A.2) one has

$$\int (\beta-h|\hat{n}|\beta'-h)\,\phi_{h,m}(\beta')\,d\beta' = \lambda_m(h)\;\phi_{h,m}(\beta) \tag{A.3}$$

where

$$(\beta-h|\hat{n}|\beta'-h) = \langle 0|\, e^{-i(\beta-h)\hat{Q}}\,\delta(\hat{P})\, e^{i(\beta'-h)\hat{Q}}\,|0\rangle$$

$$= \frac{1}{2\pi}\int d\alpha\, \langle \beta-h,\alpha|0,\beta'-h\rangle \tag{A.4}$$

The equation (A.3) yields

$$\phi_{k,n}(p) = \phi_n(p-k)$$

and $\lambda_n(k)$ independent of k .

The reduced kernel $\hat{n}$ is an hermitian, semi-positive definite Hilbert-Schmidt kernel. That it is hermitian is obvious. It is semi-positive definite because it has the same eigenvalues of the semi-positive definite kernel $\hat{N}$. Finally it is of the Hilbert Schmidt type since

$$\mathrm{tr}\,\hat{n} = 1 \tag{A.5}$$

and as $\hat{n}$ is semi-positive definite

$$\mathrm{tr}\,\hat{n}^2 \leq (\mathrm{tr}\,\hat{n})^2 \leq 1 \tag{A.6}$$

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